

=> s mutilin
L21 47 MUTILIN

=> d

L21 ANSWER 1 OF 47 REGISTRY COPYRIGHT 2008 ACS on STN

RN 1018331-67-3 REGISTRY

ED Entered STN: 30 Apr 2008

CN INDEX NAME NOT YET ASSIGNED

OTHER NAMES:

CN 14-O-[[[(S)-N-Boc-piperidin-3-yl]thio]acetyl]mutilin

methanesulfonate

CN 22-[[[(S)-N-Boc-piperidin-3-yl]thio]pleuromutilin methanesulfonate

FS STEREOSEARCH

MF C32 H51 N O6 S . C H4 O3 S

SR CA

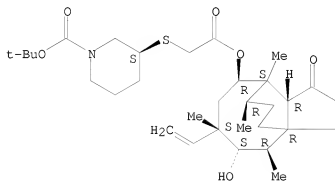
LC STN Files: CA, CAPLUS, CASREACT

CM 1

CRN 1018331-66-2

CMF C32 H51 N O6 S

Absolute stereochemistry.



CM 2

CRN 75-75-2

CMF C H4 O3 S



1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> fil caplus		
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FULL ESTIMATED COST	8.07	1359.62
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-78.40

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 FILE LAST UPDATED: 22 May 2008 (20080522/ED)

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<http://www.cas.org/legal/infopolicy.html>

=> s 12

L22 22 L2

=> d 1-22 bib abs hitstr

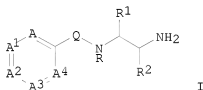
L22 ANSWER 1 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
 AN 2007:63581 CAPLUS <<LOGINID:20080523>>
 DN 146:156259
 TI MAO-B inhibitors useful for treating obesity
 IN McElroy, John F.; Chorvat, Robert J.; Rajagopalan, Parthasarathi
 PA Jenrin Discovery, USA
 SO PCT Int. Appl., 92pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----		-----	-----	-----
PI	WO 2007008963	A1	20070118	WO 2006-US27019	20060712

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

US 20070015734 A1 20070118 US 2006-456912 20060712
 PRAI US 2005-698867P P 20050713
 OS MARPAT 146:156259
 GI



AB The invention provides novel compds. of formula I (where A, A1, A2, A3, and A4, are independently selected from CH, substituted C, N, and N+O-, provided that from 0-1 is N+O-; R is independently selected from H and C1-6 alkyl; R1 is selected from H and C1-6 alkyl; R2 is selected from H and C1-6-alkyl; Q is selected from C=O and SO2) that are monoamine oxidase-B (MAO-B) inhibitors, which can be useful in treating obesity, diabetes, and/or cardiometabolic disorders (e.g., hypertension, dyslipidemias, high blood pressure, and insulin resistance).

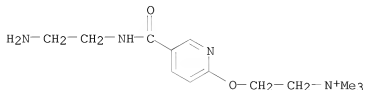
IT 919773-61-8

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(MAO-B inhibitors useful for treating obesity and other disorders)

RN 919773-61-8 CAPLUS

CN Ethanaminium, 2-[[5-[[[(2-aminoethyl)amino]carbonyl]-2-pyridinyl]oxy]-N,N,N-trimethyl-, chloride (1:1) (CA INDEX NAME)

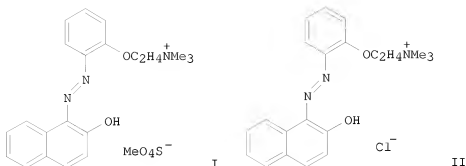


● Cl⁻

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:1004830 CAPLUS <<LOGINID:20080523>>
DN 143:287907
TI Cationic naphthylidazo dyes and colorants for keratin fibers containing
said compounds.
IN Goettel, Otto; Hayoz, Andre; Braun, Hans-Juergen
PA Wella Aktiengesellschaft, Germany
SO PCT Int. Appl., 48 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005085362	A1	20050915	WO 2004-EP14189	20041213
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SI, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	DE 102004010999	A1	20050922	DE 2004-102004010999	20040306
	EP 1740657	A1	20070110	EP 2004-803818	20041213
	EP 1740657	B1	20070912		
	R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
	BR 2004018613	A	20070502	BR 2004-18613	20041213
	AT 373051	T	20070915	AT 2004-803818	20041213
	JP 2007527457	T	20070927	JP 2007-501128	20041213
	ES 2294565	T3	20080401	ES 2004-803818	20041213
PRAI	DE 2004-102004010999	A	20040306		
	WO 2004-EP14189	W	20041213		
OS	MARPAT 143:287907				
GI					



AB Cationic naphthylidazo dyes such as, an example I or II useful for non-oxidative dyeing keratin fibers, especially hair are prepared by catalytic hydriding of nitrocompounds followed by a standard diazotization in water and coupling with 1- or 2-naphthols. Thus, I prepared by reduction of 34 g N,N,N-trimethyl-2-(2-nitrophenoxy)ethanaminium methylsulfate with H₂ (pressure 9 bar) in the presence of Pd/C catalyst followed by a standard diazotization in water with NaNO₂ and sulfamic acid and coupling with a solution of 2-naphthol in i-PrOH was used in a composition for dyeing hair

containing

4.0 g of decyl glucoside, 5.0 g of ethanol and 0.0025 mol of this dye in 100 g of water at pH 7.

IT 864465-41-8P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(diazo component precursor, nitro-compound; cationic naphthylidazo dyes useful for non-oxidative dyeing keratin fibers prepared by catalytic hydriding of nitrocompounds followed by a standard diazotization in water and coupling)

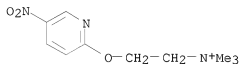
RN 864465-41-8 CAPLUS

CN Ethanaminium, N,N,N-trimethyl-2-[(5-nitro-2-pyridinyl)oxy]-, methyl sulfate (1:1) (CA INDEX NAME)

CM 1

CRN 864465-40-7

CMF C10 H16 N3 O3



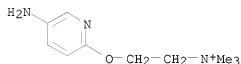
CM 2

CRN 21228-90-0

CMF C H3 O4 S



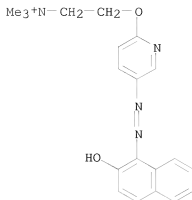
IT 864465-43-0P
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT
 (Reactant or reagent)
 (diaz component; cationic naphthylidazo dyes useful for non-oxidative
 dyeing keratin fibers prepared by catalytic hydriding of nitrocompounds
 followed by a standard diazotization in water and coupling)
 RN 864465-43-0 CAPLUS
 CN Ethanaminium, 2-[(5-amino-2-pyridinyl)oxy]-N,N,N-trimethyl-, methyl
 sulfate (1:1) (CA INDEX NAME)
 CM 1
 CRN 864465-42-9
 CMF C10 H18 N3 O



CM 2
 CRN 21228-90-0
 CMF C H3 O4 S



IT 864465-26-9P
 RL: COS (Cosmetic use); IMF (Industrial manufacture); BIOL (Biological
 study); PREP (Preparation); USES (Uses)
 (orange dye; cationic naphthylidazo dyes useful for non-oxidative
 dyeing keratin fibers prepared by catalytic hydriding of nitrocompounds
 followed by a standard diazotization in water and coupling)
 RN 864465-26-9 CAPLUS
 CN Ethanaminium, 2-[[5-[2-(2-hydroxy-1-naphthalenyl)diazonyl]-2-
 pyridinyl]oxy]-N,N,N-trimethyl-, chloride (1:1) (CA INDEX NAME)



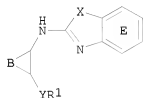
● Cl⁻

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

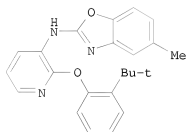
L22 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:696902 CAPLUS <<LOGINID::20080523>>
DN 143:194003
TI Preparation of aminobenzazoles and analogs as P2Y1 receptor inhibitors for
treating thromboembolic disorders
IN Herpin, Timothy F.; Morton, George C.; Rehfuess, Robert P.; Lawrence, R.
Michael; Poss, Michael A.; Roberge, Jacques Y.; Gungor, Timur
PA Bristol-Myers Squibb Company, USA
SO PCT Int. Appl., 256 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005070920	A1	20050804	WO 2005-US1705	20050120
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, GU, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 20050203146	A1	20050915	US 2005-38862	20050119
EP 1706398	A1	20061004	EP 2005-711663	20050120
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK,			

	HR, IS, YU				
	JP 2007518809	T	20070712	JP 2006-551237	20050120
	NO 2006003191	A	20061016	NO 2006-3191	20060710
PRAI	US 2004-537869P	P	20040121		
	US 2004-638167P	P	20041222		
	WO 2005-US1705	W	20050120		
OS	MARPAT 143:194003				
GI					

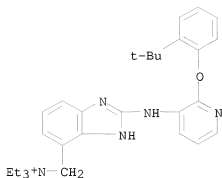


I



II

- AB The invention is related to novel aminobenzazoles I and their analogs, and their stereoisomers, pharmaceutically acceptable salts and solvates [wherein B = (un)substituted Ph, heteroaryl; E = (un)substituted Ph, pyridinyl, pyrimidinyl, pyrazinyl, pyridazinyl; X = NH and derivs., O, S; Y = O, S, SO, SO₂; R₁ = (un)substituted carbocyclyl, heterocyclyl] as selective inhibitors of the human P2Y₁ receptor. For example, II was prepared by reacting 2-[(2-tert-butylphenyl)oxy]-3-isothiocyanatopyridine (preparation given) with 2-amino-p-cresol, followed by cyclization. Preferred I have K_i's ≤ 1 μM in a P2Y₁ binding assay. I, and their pharmaceutical compns., are useful for treating diseases responsive to modulation of P2Y₁ receptor activity, especially thromboembolic disorders.
- IT 861672-42-6P, N-[[2-[[2-[(2-tert-Butylphenyl)oxy]pyridin-3-yl]amino]-3H-benzo[d]imidazol-4-yl]methyl]-N,N-diethylethanaminium chloride
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (drug candidate; preparation of aminobenzazoles and analogs as P2Y₁ receptor inhibitors for treating thromboembolic disorders)
- RN 861672-42-6 CAPLUS
- CN 1H-Benzimidazole-7-methanaminium, 2-[[2-[(2-(1,1-dimethylethyl)phenoxy]-3-pyridinyl]amino]-N,N,N-triethyl-, chloride (1:1) (CA INDEX NAME)

● Cl⁻

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 4 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2004:60147 CAPLUS <<LOGINID::20080523>>

DN 140:111291

TI Preparation of substituted 5-aryl-benzothiepinines as ileal bile acid transport and taurocholate uptake inhibitors

IN Lee, Len F.; Banerjee, Shyamal C.; Huang, Horng Chih; Li, Jinglin J.; Miller, Raymond E.; Reitz, David B.; Tremont, Samuel J.

PA G.D. Searle and Co., USA

SO U.S. Pat. Appl. Publ., 235 pp., Cont.-in-part of U.S. Ser. No. 831,284.

CODEN: USXXCO

DT Patent

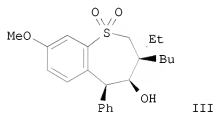
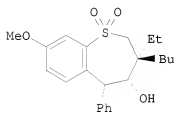
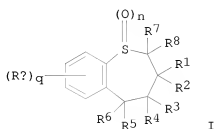
LA English

FAN.CNT 9

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 20040014803	A1	20040122	US 2002-68297	20020208
	US 6784201	B2	20040831		
	CA 2506703	A1	19970918	CA 1997-2506703	19970311
	EP 1440972	A1	20040728	EP 2004-10088	19970311
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
	AU 761249	B2	20030529	AU 2000-53394	20000816
	US 20020013476	A1	20020131	US 2001-828968	20010409
	US 6387924	B2	20020514		
	US 20030171426	A1	20030911	US 2002-76091	20020215
	US 6642268	B2	20031104		
	AU 2003201377	A1	20030612	AU 2003-201377	20030318
	US 20040204478	A1	20041014	US 2004-830125	20040423
PRAI	US 1994-305526	B2	19940913		
	US 1995-517051	B1	19950821		
	US 1996-13119P	P	19960311		
	US 1997-816065	A2	19970311		
	US 1997-831284	A2	19970331		

US 2001-828968	A3	20010409
AU 1997-23266	A3	19970311
CA 1997-2248586	A3	19970311
EP 1997-915976	A3	19970311
US 1997-40660P	P	19970311
US 1997-68170P	P	19971219
US 1998-109551	A2	19980702
US 1999-275463	A1	19990324
US 1999-443403	A1	19991119
AU 2000-53394	A3	20000816
US 2000-676466	A3	20000929
US 2002-68297	A3	20020208

OS
GI MARPAT 140:111291



AB The title compds. (I) [wherein q = 1-4; n = 0-2; R1, R2 = H, (un)substituted (halo)alkyl, alkenyl, alkynyl, alkylaryl, arylalkyl, alkoxy(alkyl), dialkylamino, alkylthio, (polyalkyl)aryl, or cycloalkyl; or R1 and R2 taken together with the atoms to which they are attached = cycloalkyl; R3, R4 = H, alkyl, alkenyl, alkynyl, acyloxy, aryl, heterocyclyl, OR9, NR9R10, SR9, S(O)R9, SO2R9, or SO3R9; R9, R10 = H, (cyclo)alkyl, alkenyl, alkynyl, aryl(alkyl), acyl, heterocyclyl, or ammoniumalkyl; or R3 and R4 together = :O, :NOR11, :S, :NNR11R12, :NR9, or :CR11R12; R11, R12 = H, (cyclo)alkyl, alkenyl, alkynyl, aryl(alkyl), heterocyclyl, carboxylalkyl, carboalkoxyalkyl, cyanoalkyl, OR9, NR9R10, SR9, S(O)R9, SO2R9, SO3R9, CO2R9, CN, halo, oxo, or CONR9R10; R5, R6 = H, alkyl, aryl, etc.; R7, R8 = H, alkyl; Rx = H, (un)substituted (cyclo)alkyl, alkenyl, alkynyl, polyalkyl, acyloxy, aryl(alkyl), halo(alkyl), (quaternary) heterocyclyl, (quaternary) heteroaryl, polyether, alkoxy, amino, alkylthio, NO2, carboxy, carbamido, etc.] were prepared for the prophylaxis and treatment of hyperlipidemic conditions, such as those associated with atherosclerosis or hypercholesterolemia. Thus, KOBu-t was added to a solution of 2-(2-benzyl-5-

methoxyphenylsulfonyl)methyl)-2-ethylhexanal (preparation given) and dry THF cooled to -1.6°C to give, after workup, II and III (96% combined yield). The isomers were separated upon recrystn. II inhibited IBAT-mediated uptake of [14C]-taurocholate in H14 cells with an IC50 of 0.1 µM and reduced serum cholesterol from 143 mg (7%) to 126 mg (2%) compared to control in cholesterol-fed hamsters in a 14-day test. In vitro taurocholate uptake assay data are included for nearly 600 compds. of the invention.

IT 289038-40-0P

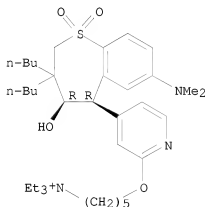
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(hypolipemic agent; preparation of substituted 5-aryl-benzothiepinines by cyclization of 2-((2-benzyl- and 2-benzoylphenylthio)methyl)alkanals as ileal bile acid transport and taurocholate uptake inhibitors)

RN 289038-40-0 CAPLUS

CN 1-Pentanaminium, 5-[[4-[(4R,5R)-3,3-dibutyl-7-(dimethylamino)-2,3,4,5-tetrahydro-4-hydroxy-1,1-dioxido-1-benzothiepin-5-yl]-2-pyridinyl]oxy]-N,N,N-triethyl-, iodide, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



● I⁻

RE.CNT 231 THERE ARE 231 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 5 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2003:692092 CAPLUS <<LOGINID::20080523>>

DN 139:270263

TI Quaternary ammonium 3-(aminoethoxy)pyridines as antinociceptive agents

AU Simsek, Rahime; Chang-Fong, Jean; Lee, Mase; Dukat, Malgorzata; Damaj, M. Imad; Martin, Billy R.; Glennon, Richard A.

CS Department of Medicinal Chemistry, School of Pharmacy, Virginia Commonwealth University, Richmond, VA, 23298, USA

SO Bioorganic & Medicinal Chemistry Letters (2003), 13(17), 2917-2920

CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science B.V.

DT Journal

LA English

AB Quaternization via N-methylation of the terminal amines of a series of 3-(dialkylaminoethoxy)pyridines resulted in analogs that displayed up to 50-60-fold enhanced affinity for nicotinic acetylcholinergic (nACh) receptors. Several of these compds. displayed antinociceptive properties in mice using the tail-flick assay and serve as possible leads for the development of novel analgesic agents.

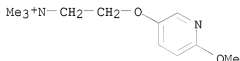
IT 607390-42-1

RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(quaternary ammonium 3-(aminoethoxy)pyridines as nicotinic agonists and antinociceptive agents)

RN 607390-42-1 CAPLUS

CN Ethanaminium, 2-[(6-methoxy-3-pyridinyl)oxy]-N,N,N-trimethyl-, chloride (1:1) (CA INDEX NAME)

● Cl⁻

RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 6 OF 22 CAPLUS COPYRIGHT 2008 ACS ON STN

AN 2000:590035 CAPLUS <<LOGINID::20080523>>

DN 133:193089

TI Preparation of substituted 5-aryl-benzothiepinines as ileal bile acid transport and taurocholate uptake inhibitors

IN Lee, Len F.; Banerjee, Shyamal C.; Huang, Horng-chih; Li, Jinglin J.; Miller, Raymond E.; Reitz, David B.; Tremont, Samuel J.

PA G.D. Searle and Co., USA

SO U.S., 191 pp., Cont.-in-part of U. S. Ser. No. 109,551.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 9

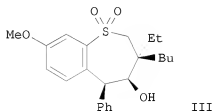
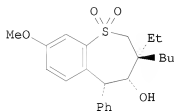
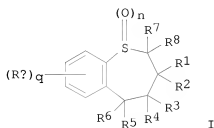
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PI	US 6107494	A	20000822	US 1999-275463	19990324
	CA 2506703	A1	19970918	CA 1997-2506703	19970311
	EP 1440972	A1	20040728	EP 2004-10088	19970311
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	US 5994391	A	19991130	US 1998-109551	19980702
	EP 1331225	A1	20030730	EP 2003-5459	19981216

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CA 2336315	A1	20000113	CA 1999-2336315 19990629
WO 2000001687	A1	20000113	WO 1999-US12828 19990629
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AU 9948202	A	20000124	AU 1999-48202 19990629
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US 6262277	B1	20010717	US 1999-443403 19991119
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US 1999-275463	A1	19990324
EP 1999-931769	A3	19990629
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US 2000-581897	A3	20001002
US 2001-828968	A3	20010409
US 2002-68297	A3	20020208

OS MARPAT 133:193089

GI



AB The title compds. (I) [wherein q = 1-4; n = 2; R1 and R2 = independently H or (un)substituted (halo)alkyl, alkenyl, alkynyl, alkylaryl, arylalkyl, alkoxy(alkyl), dialkylamino, alkylthio, (polyalkyl)aryl, or cycloalkyl; or R1 and R2 taken together with the atoms to which they are attached = cycloalkyl; R3 and R4 = independently H, alkyl, alkenyl, alkynyl, acyloxy, aryl, heterocyclyl, OR9, NR9R10, SR9, S(O)R9, SO2R9, or SO3R9; R9 and R10 = independently H, (cyclo)alkyl, alkenyl, alkynyl, aryl(alkyl), acyl, heterocyclyl, or ammoniumalkyl; or R3 and R4 together = :O, :NR11, :S, :NRR11R12, :NR9, or :CR11R12; R11 and R12 = independently H, (cyclo)alkyl, alkenyl, alkynyl, aryl(alkyl), heterocyclyl, carboxylalkyl, carboalkoxyalkyl, cyanoalkyl, OR9, NR9R10, SR9, S(O)R9, SO2R9, SO3R9, CO2R9, CN, halo, oxo, or CONR9R10; R5 = substituted aryl; R6 = H; R7 and

R8 = independently H or alkyl; Rx = independently H or (un)substituted (cyclo)alkyl, alkenyl, alkynyl, polyalkyl, acyloxy, aryl(alkyl), halo(alkyl), (quaternary) heterocyclyl, (quaternary) heteroaryl, polyether, alkoxy, amino, alkylthio, NO₂, carboxy, carbamido, etc.] where prepared for the prophylaxis and treatment of hyperlipidemic conditions, such as those associated with atherosclerosis or hypercholesterolemia. Thus, KOBu-t was added to a solution of 2-((2-benzyl-5-methoxyphenylsulfonyl)methyl)-2-ethylhexanal (preparation given) and dry THF cooled to -1.6°C to give, after workup, II and III (96% combined yield). The isomers were separated upon recrystn. II inhibited IBAT-mediated uptake of [14C]-taurocholate in H14 cells with an IC₅₀ of 0.1 μM and reduced serum cholesterol from 143 mg (7%) to 126 mg (2%) compared to control in cholesterol-fed hamsters in a 14-day test. In vitro taurocholate uptake assay data are included for nearly 600 compds. of the invention.

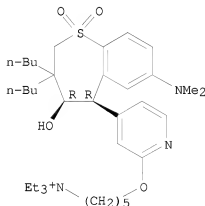
IT 289038-40-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(hypolipemic agent; preparation of substituted 5-aryl-benzothiepinines by cyclization of 2-((2-benzyl- and 2-benzoylphenylthio)methyl)alkanals as ileal bile acid transport and taurocholate uptake inhibitors)

RN 289038-40-0 CAPLUS

CN 1-Pentanaminium, 5-[[4-[(4R,5R)-3,3-dibutyl-7-(dimethylamino)-2,3,4,5-tetrahydro-4-hydroxy-1,1-dioxido-1-benzothiepin-5-yl]-2-pyridinyl]oxy]-N,N,N-triethyl-, iodide, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



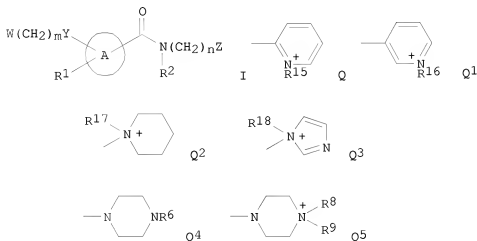
● I⁻

RE.CNT 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L22 ANSWER 7 OF 22 CAPLUS COPYRIGHT 2008 ACS ON STN
AN 1999:206866 CAPLUS <<LOGINID::20080523>>

DN 130:291600
 TI Amides, bone formation promoters containing them, and their use as
 antiosteoporotic agents
 IN Shibata, Saizo; Omori, Fujimi; Nakagawa, Takashi
 PA Japan Tobacco, Inc., Japan
 SO Jpn. Kokai Tokkyo Koho, 45 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 11080107	A	19990326	JP 1997-251360	19970901
PRAI	JP 1997-251360		19970901		
OS	MARPAT 130:291600				
GI					



AB Bone formation promoters contain amides I [W = H, amino, NHCOR3 (R3 = lower alkyl), lower alkoxy, carbonyl, cycloalkyl, naphthyl, morpholino, thienyl, phthalimido, benzoyl, benzyloxy, C6H4R4 (R4 = H, halo, lower alkyl, lower alkoxy); Y = O, NHCOR3, NHCO, CONH, CO, CO2, OCO, CO(CH:CH)u (u = 1, 2), direct bond; ring A = benzene, naphthalene, cyclohexane, biphenyl, di-Ph ether, pyridine, isoxazole, thiophene; R1 = H, halo, NO2, lower alkyl, lower alkoxy; R2 = H, lower alkyl; Z = halo, OH, lower alkyl, lower alkoxy, lower alkoxy, carbonyl, carboxy, NR5R6 (R5, R6 = H, (hydroxy)alkyl, aryl, lower alkyl, carbonyl), N+R7R8R9 (R7, R8 = lower alkyl, aralkyl; R9 = lower alkyl, (halo)aralkyl, aryl, carbonyl, alkyl), SR10 (R10 = lower alkyl, aralkyl), SO2R11 (R11 = lower alkyl, aralkyl), SOR12 (R12 = lower alkyl, aralkyl), S+R13R14 (R13, R14 = lower alkyl), morpholino, pyridyl, pyridinio, Q (R15 = lower alkyl), Q1 (R16 = lower alkyl), Q2 (R17 = lower alkyl), Q3 (R18 = lower alkyl); R2 and R5 may be bonded to each other to form Q4 (R6 = any group given above); R2 and R7

may be bonded to each other to form Q5 (R8, R9 = any group given above), m = 0-20; n = 0-4] or their pharmaceutically acceptable salts as active ingredients. Pharmaceutical compns. and antiosteoporotic agents containing I or their salts are also claimed. N-[2-(dimethylamino)ethyl]4-(nonyloxy)benzamide hydrochloride (preparation given) at 3 μ M showed 244% osteoblast growth promoting activity.

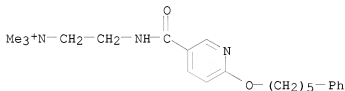
IT 222980-28-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of (hetero)aromatic amides as bone formation promoters for treatment of osteoporosis)

RN 222980-28-1 CAPLUS

CN Ethanaminium, N,N,N-trimethyl-2-[[[6-[(5-phenylpentyl)oxy]-3-pyridinyl]carbonyl]amino]-, iodide (9CI) (CA INDEX NAME)



L22 ANSWER 8 OF 22 CAPLUS COPYRIGHT 2008 ACS ON STN

AN 1995:994323 CAPLUS <<LOGINID::20080523>>

DN 124:31986

OREF 124:6095a,6098a

TI Cationically bridged tetrakisazo dyes, their preparation and use

IN Moser, Helmut Anton

PA Sandoz Ltd., Switz.

SO Brit. UK Pat. Appl., 31 pp.

CODEN: BAXXDU

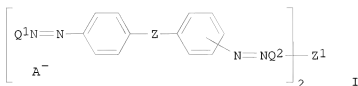
DT Patent

LA English

FAN.CNT 1

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	DE 19500203	A1	19950720	DE 1995-19500203	19950105
	FR 2715159	A1	19950721	FR 1995-232	19950109
	ES 2111449	A1	19980301	ES 1995-37	19950111
	ES 2111449	B1	19990701		
	CH 688552	A5	19971114	CH 1995-91	19950112
	US 5545724	A	19960813	US 1995-540528	19950101
PRAI	DE 1994-4400855	A	19940114		
	US 1995-371727	B1	19950112		

OS MARPAT 124:31986
GI



AB The cationically bridged tetrakisazo compds. correspond to formula I, in which A1 is an anion, preferably of a carboxylic acid, Q1 is a coupling agent residue, Q2 is the residue of a cationic pyridone coupler or a pyridone coupler carrying a tertiary amino group, Z is a bridging group, and Z1 is hydroxyalkylene, alkylene, or xylylene. Each disazo chromophore contains ≥ 2 water-solubilizing groups and coupling must be asym. The compds. and their preps. are used for dyeing and printing OH group-containing or N-containing organic substrates by known methods.

Preferred substrates are textile materials which consist of or contain cellulose, especially cotton or bast fibers, leather, and paper or pulp products. Thus, 4-H2NC6H4CONHC6H4NH2-4 was tetrazotized and coupled consecutively with N-(1,2-dihydro-6-hydroxy-4-methyl-2-oxo-3-pyridyl)-3-methylpyridinium chloride at pH 0.5-2 and 1-[3-(dimethylamino)propyl]-6-hydroxy-4-methyl-2-pyridinone to give a disazo compound, which was coupled 2:1 by quaternization with (ClCH2)2CHOH to give a product which dyes paper yellow.

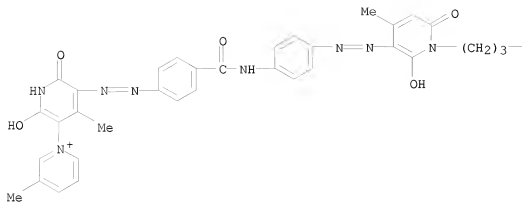
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171848-57-0P 171848-59-2P 171848-60-5P
171849-01-7P 171849-02-8P 171849-04-0P
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(yellow; cationically bridged tetrakisazo dyes for cellulosic substrates and leather)

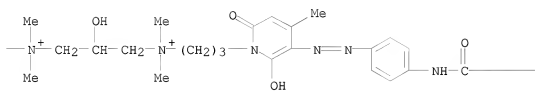
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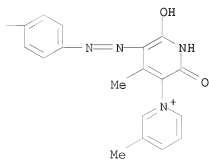
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● 4 OH⁻

PAGE 1-B

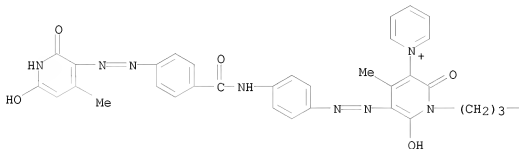


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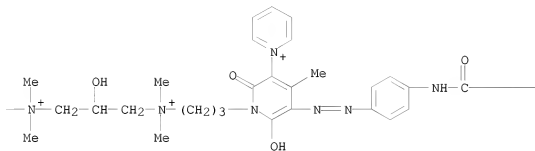


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 CN 1,3'-Bipyridinium, 5',5'''-[(2-hydroxy-1,3-propanediyl)bis[(dimethyliminio)-3,1-propanediyl]]bis[5'-[[4-[[4-[(1,2-dihydro-6-hydroxy-4-methyl-2-oxo-3-pyridinyl)azo]benzoyl]amino]phenyl]azo]-6'-hydroxy-4'-methyl-2'-oxo-, tetrahydroxide (9CI) (CA INDEX NAME)

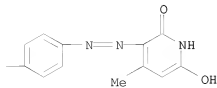
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PAGE 1-B

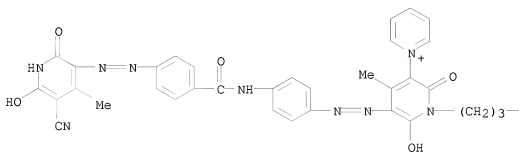


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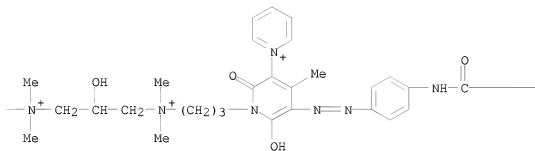
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PAGE 1-A

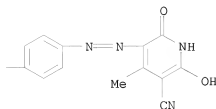


● 4 OH⁻

PAGE 1-B

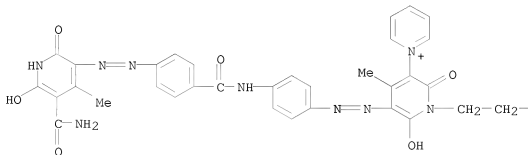


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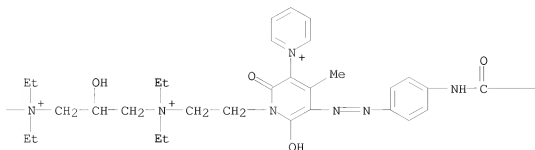


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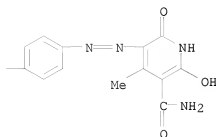
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● 4 OH⁻

PAGE 1-B

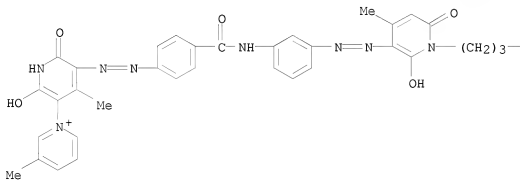


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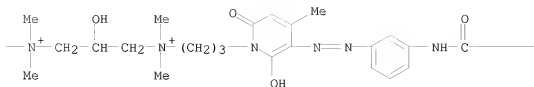
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PAGE 1-A

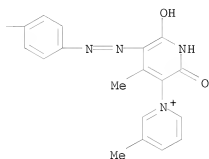


● 4 OH⁻

PAGE 1-B

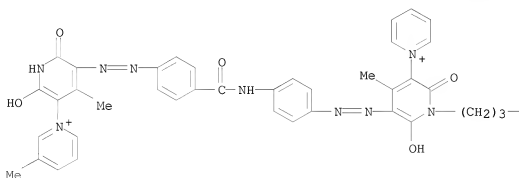


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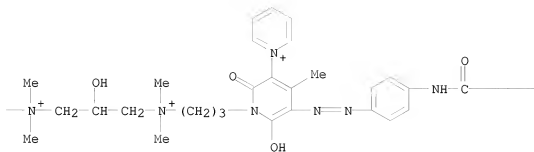
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 CN 1,3'-Bipyridinium, 1',1'''-[(2-hydroxy-1,3-propanediyl)bis[(dimethyliminio)-3,1-propanediyl]]bis[5'-[[4-[[4-[(1',2'-dihydro-6'-hydroxy-4'-methyl-2'-oxo[1,3'-bipyridinium]-5'-yl)azo]benzoyl]amino]phenyl]azo]-1',2'-dihydro-6'-hydroxy-4'-methyl-2'-oxo-, hexahydroxide (9CI) (CA INDEX NAME)

PAGE 1-A

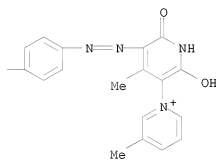


● 6 OH⁻

PAGE 1-B

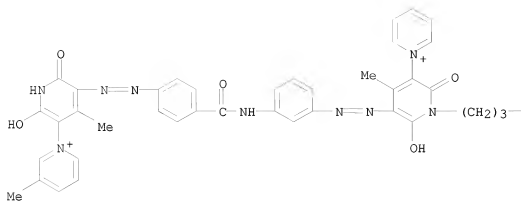


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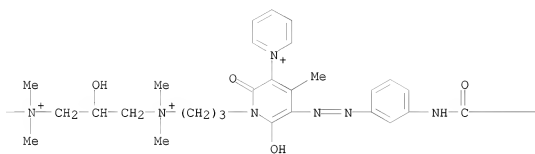


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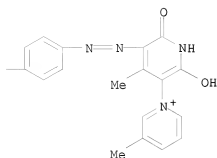
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PAGE 1-B

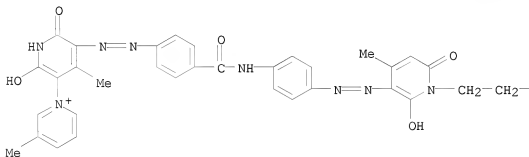


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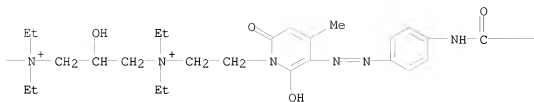
RN 171848-55-8 CAPLUS
 CN 1,3'-Bipyridinium, 5',5'''-[(2-hydroxy-1,3-propanediyl)bis[(diethyliminio)-2,1-ethanediyl(2-hydroxy-4-methyl-6-oxo-1,3(6H)-pyridinediyl)azo-4,1-phenyleneiminocarbonyl-4,1-phenyleneazo]]bis[1',2'-dihydro-6'-hydroxy-3,4'-dimethyl-2'-oxo-, tetrahydroxide (9CI) (CA INDEX NAME)

PAGE 1-A

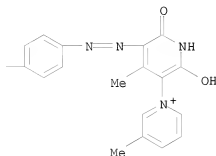


● 4 OH⁻

PAGE 1-B



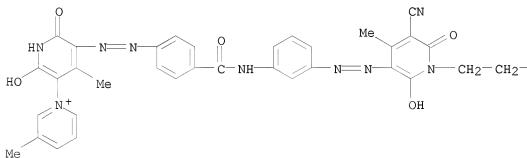
PAGE 1-C



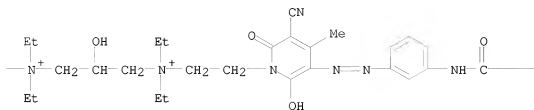
RN 171848-56-9 CAPLUS

CN 1,3'-Bipyridinium, 5',5'''-[(2-hydroxy-1,3-propanediyl)bis[(diethyliminio)-2,1-ethanediyl(5-cyano-2-hydroxy-4-methyl-6-oxo-1,3(2H)-pyridinediyl)azo-3,1-phenyleneiminocarbonyl-4,1-phenyleneazo]]bis[1',2'-dihydro-6'-hydroxy-3,4'-dimethyl-2'-oxo-, tetrahydroxide (9CI) (CA INDEX NAME)

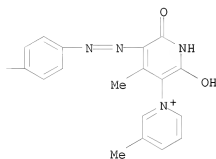
PAGE 1-A

● 4 OH⁻

PAGE 1-B

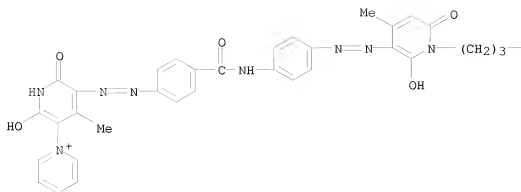


PAGE 1-C

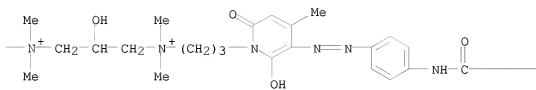


RN 171848-57-0 CAPLUS
 CN 1,3'-Bipyridinium, 5',5'''-[(2-hydroxy-1,3-propanediyl)bis[(dimethyliminio)-3,1-propanediyl(2-hydroxy-4-methyl-6-oxo-1,3 (2H)-pyridinediyl)azo-4,1-phenyleneimino-carbonyl-4,1-phenyleneazo]]bis[1',2'-dihydro-6'-hydroxy-4'-methyl-2'-oxo-, tetrahydroxide (9CI) (CA INDEX NAME)

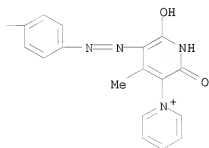
PAGE 1-A



PAGE 1-B



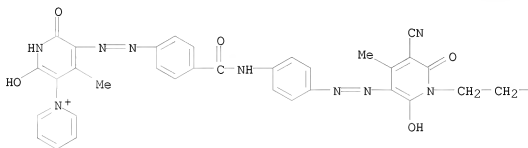
PAGE 1-C



RN 171848-59-2 CAPLUS

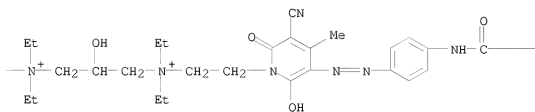
CN 1,3'-Bipyridinium, 5',5'''-[(2-hydroxy-1,3-propanediyl)bis[(diethyliminio)-2,1-ethanediyl(5-cyano-2-hydroxy-4-methyl-6-oxo-1,3(2H)-pyridinediyl)azo-4,1-phenyleneiminocarbonyl-4,1-phenyleneazo]]bis[1',2'-dihydro-6'-hydroxy-4'-methyl-2'-oxo-, tetrahydroxide (9CI) (CA INDEX NAME)

PAGE 1-A

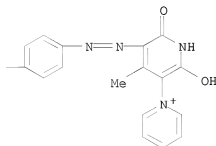


● 4 OH⁻

PAGE 1-B

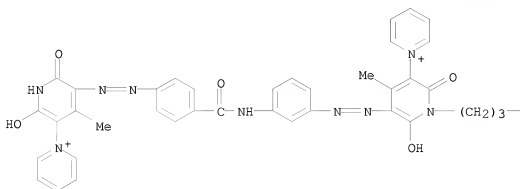


PAGE 1-C

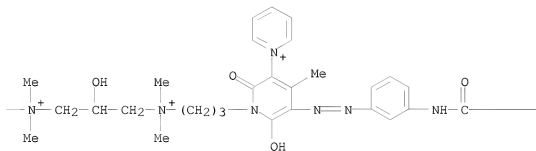


RN 171848-60-5 CAPLUS
 CN 1,3'-Bipyridinium, 1,1'''-[(2-hydroxy-1,3-propanediyl)bis[(dimethyliminio)-3,1-propanediyl]]bis[5'-[[3-[[4-[(1',2'-dihydro-6'-hydroxy-4'-methyl-2'-oxo[1,3'-bipyridinium]-5'-yl)azo]benzoyl]amino]phenyl]azo]-1',2'-dihydro-6'-hydroxy-4'-methyl-2'-oxo-, hexahydroxide (9CI) (CA INDEX NAME)

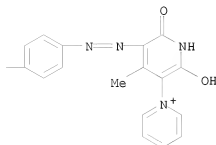
PAGE 1-A



PAGE 1-B

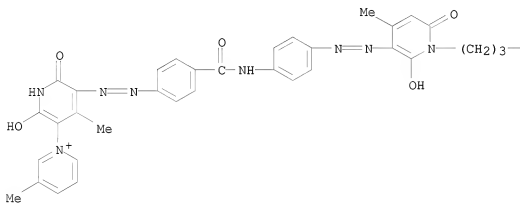


PAGE 1-C

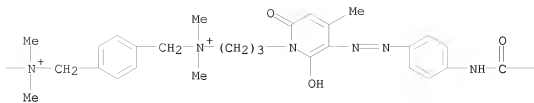


RN 171849-01-7 CAPLUS
 CN 1,3'-Bipyridinium, 5',5'''-[1,4-phenylenebis[methylene(dimethyliminio)-3,1-propanediyl(2-hydroxy-4-methyl-6-oxo-1,3(6H)-pyridinediyl)azo-4,1-phenyleneimino]bis[1',2'-dihydro-6'-hydroxy-3,4'-dimethyl-, tetrahydroxide (9CI) (CA INDEX NAME)

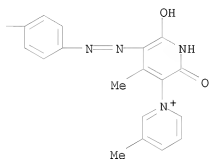
PAGE 1-A

● 4 OH⁻

PAGE 1-B



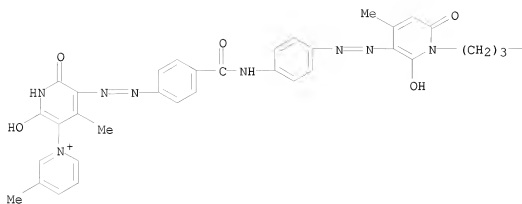
PAGE 1-C



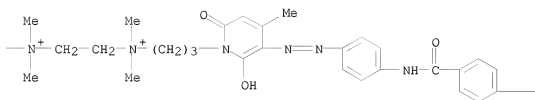
RN 171849-02-8 CAPLUS

CN 1,3'-Bipyridinium, 5',5'''-[1,2-ethanediylbis[(dimethyliminio)-3,1-propanediyl(2-hydroxy-4-methyl-6-oxo-1,3(6H)-pyridinediyl)azo-4,1-phenyleneimino-carbonyl-4,1-phenyleneazo]]bis[1',2'-dihydro-6'-hydroxy-3,4'-dimethyl-, tetrahydroxide (9CI) (CA INDEX NAME)

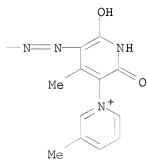
PAGE 1-A



PAGE 1-B



PAGE 1-C



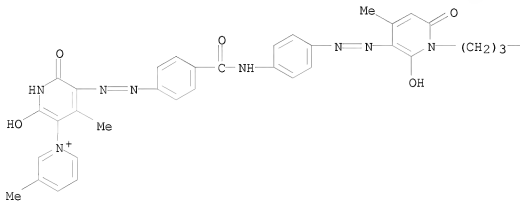
RN 171849-04-0 CAPLUS
 CN 1,3'-Bipyridinium, 5',5'''-[(2-hydroxy-1,3-propanediyl)bis[(dimethyliminio)-3,1-propanediyl(2-hydroxy-4-methyl-6-oxo-1,3(6H)-pyridinediyl)azo-4,1-phenyleneiminocarbonyl-4,1-phenyleneazo]]bis[1',2'-dihydro-6'-hydroxy-3,4'-dimethyl-, tetraacetate (salt) (9CI) (CA INDEX NAME)

CM 1

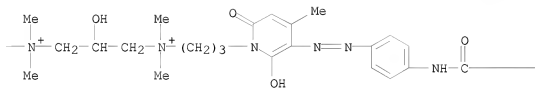
CRN 171849-03-9

CMF C75 H82 N18 O11

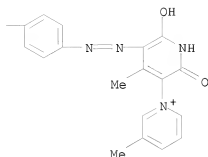
PAGE 1-A



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CM 2

CRN 71-50-1

CMF C2 H3 O2



L22 ANSWER 9 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1990:17758 CAPLUS <<LOGINID::20080523>>

DN 112:17758

OREF 112:3065a,3068a

TI Preparation of herbicidal aryloxypropionates

IN Bartha, Ferenc; Galamb, Vilmos; Repasi Veres, Agota; Timar, Tibor; Tompa, Jozsef; Fodor, Istvan; Zsupan, Kalman

PA Alkaloida Vegyeszeti Gyar, Hung.

SO Hung. Teljes, 40 pp.

CODEN: HUXXB

DT Patent

LA Hungarian

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
PI	HU 47525	A2	19890328	HU 1987-2997	19870702
PRAI	HU 1987-2997		19870702		
OS	MARPAT 112:17758				

AB The aryloxypropionates ArOCHMeCOR [Ar = aryl; R = OR1, NR2R3; R1 = alkyl, alkenyl, alkynyl (CH₂CH₂)_nNR4R5, (CH₂CH₂)_nN+R4R5R6Y-, (CH₂CH₂)_nOR7; R2 = H; R3 = alkyl, cycloalkyl, aryl, etc.; R2R3 = alkylene; R4,R5,R7 = alkyl; R6 = H, alkyl; n = 1-4; Y = anion] are prepared as optical isomers or racemic compds. by reacting the esters $\text{ArOCHMeCO}_2\text{Me}$ with RmA (R = OH, NH₂, NH-, m = 1, 2). The aryloxypropionates are herbicides. A mixture of Me

2-(2,4-dichlorophenoxy)propionate, furfurylamine and NH_4Cl was stirred for 5 h at 80° , to give 2-(2,4-dichlorophenoxy)propionic acid furfurylamide (I). Postemergence 5 kg I/ha controlled *Ambrosia elatior*, *Avena fatua*, *Echinochloa crus-galli*, and other weeds. An emulsion concentrate comprised 20% N-phosphonomethylglycine, 40 g N,N-dimethylaminoethyl 2-[4-(5-trifluoromethylpyrid-2-yloxy)phenoxy]propionate, 50 mL water, 50 mL paraffin oil and 10 g α,ω -polyethylene oxide diol.

IT 124371-94-4P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as herbicide)

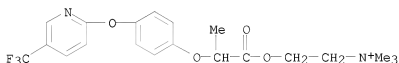
RN 124371-94-4 CAPLUS

CN Ethanaminium, N,N,N-trimethyl-2-[1-oxo-2-[4-[[5-(trifluoromethyl)-2-pyridinyl]oxy]phenoxy]propoxy]-, methanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 124371-93-3

CMF C20 H24 F3 N2 O4



CM 2

CRN 16053-58-0

CMF C H3 O3 S



L22 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1989:635621 CAPLUS <<LOGINID::20080523>>

DN 111:235621

OREF 111:39125a,39128a

TI Aggregate structure and ligand location strongly influence copper(II) binding ability of cationic metallosurfactants

AU Scrimin, Paolo; Tecilla, Paolo; Tonellato, Umberto; Vendrame, Tiziano

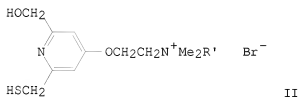
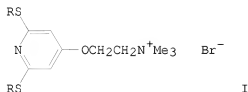
CS Dip. Chim. Org., Univ. Padova, Padova, 35131, Italy

SO Journal of Organic Chemistry (1989), 54(25), 5988-91

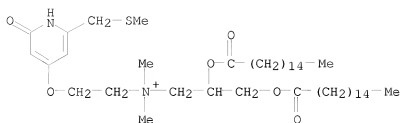
CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA English
GI



- AB Ligand surfactants I (R = octyl, lauryl, palmityl) and non-surfactant model I (R = Me) were synthesized. Their binding consts. and those of II [R' = hexadecyl or 2,3-bis(palmitoyl)propyl] with Cu(II) ions strongly depended on the structure of the aggregate (micelles or vesicles) and the location of the ligand subunit (micelles or vesicles) and the location of the ligand subunit (inside or outside the membrane). Micelles were not sensitive to the position of the coordinating moiety, while vesicles show no detectable binding of Cu(II) ions when the coordination site was inside the vesicular membrane [as in I [R = lauryl, palmityl]]. The observed effects were attributed to the high order of the hydrocarbon chains in the vesicles, which precluded the binding site modification required for the complexation process, as well as to the very high hydrophobicity of the bilayer.
- IT 122899-70-1
RL: USES (Uses)
(copper-binding properties of, micellar and vesicular structure effect on)
- RN 122899-70-1 CAPLUS
- CN 1-Propanaminium, N-[2-[[1,2-dihydro-6-[(methylthio)methyl]-2-oxo-4-pyridinyl]oxy]ethyl]-N,N-dimethyl-2,3-bis[(1-oxohexadecyl)oxy]-, bromide (9CI) (CA INDEX NAME)



● Br⁻

L22 ANSWER 11 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1984:53193 CAPLUS <<LOGINID::20080523>>

DN 100:53193

OREF 100:8137a,8140a

TI Basic and/or cationic pyridinone-containing dis- or polyazo dyes

IN Greve, Manfred; Moser, Helmut; Pedrazzi, Reinhard; Wald, Roland

PA Sandoz-Patent-G.m.b.H., Fed. Rep. Ger.

SO Ger. Offen., 36 pp.

CODEN: GWXXBX

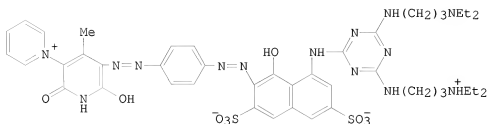
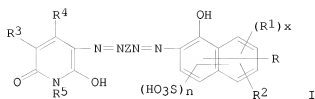
DT Patent

LA German

FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 3213826	A1	19831027	DE 1982-3213826	19820415
	EP 92520	A2	19831026	EP 1983-810152	19830413
	EP 92520	A3	19831130		
	EP 92520	B1	19861112		
	R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
	AT 23551	T	19861115	AT 1983-810152	19830413
	CA 1211751	A1	19860923	CA 1983-425900	19830414
	JP 58213052	A	19831210	JP 1983-65743	19830415
	JP 03056595	B	19910828		
	BR 8301953	A	19831220	BR 1983-1953	19830415
	ZA 8302675	A	19841128	ZA 1983-2675	19830415
	US 4673735	A	19870616	US 1984-598236	19840409
	US 4780106	A	19881025	US 1987-61076	19870610
PRAI	DE 1982-3213826	A	19820415		
	DE 1983-3302614	A	19830127		
	DE 1983-3302950	A	19830129		
	EP 1983-810152	A	19830413		
	US 1983-485212	A2	19830415		
	DE 1983-3316915	A	19830509		
	US 1984-598236	A3	19840409		

GI



IV

AB Title dyes of general structure I are prepared, where Z = tetrazo component residue, optionally containing a bridging moiety; R = H or benzoylamino or (triazinylamino)benzoylamino containing a diamine or quaternized diamine residue as a substituent; R1 = azo or disazo substituent; x = 0 or 1 (R = H when x = 1); R2 = H, OH, NH2, etc.; n = 0, 1 or 2 (but at least one less than the total number of basic and/or cation groups); R3 = H, halogen, carbamoyl, etc.; R4 = H, OH, alkyl, Ph, etc.; and R5 = H, hydroxyalkyl, Ph, cycloalkyl, etc. I and their metal complexes are fast dyes for cellulosic substrates (especially paper) and leather. Thus, diazotization of 5-[(4-aminophenyl)azo]-6-hydroxy-4-methyl-3-pyridinio-2-pyridone chloride (II) [88341-91-7] and coupling with 1-[[4,6-bis[[3-(diethylamino)propyl]amino]-s-triazin-2-yl]amino]-8-hydroxy-3,6-naphthalenedisulfonic acid (III) [88341-90-6] (synthesis of II and III described) gave IV [88341-85-9], a blue dye exhibiting high wetfastness on paper when applied as an acid addition salt. Numerous other I are reported, and dyeing examples are given.

IT 88470-75-1 88470-78-4

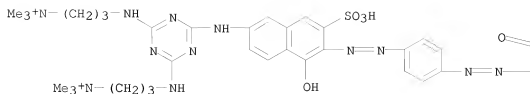
RL: USES (Uses)

(dye, for paper)

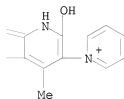
RN 88470-75-1 CAPLUS

CN 1,3'-Bipyridinium, 5'-[[4-[[6-[[4,6-bis[[3-(trimethylammonio)propyl]amino]-1,3,5-triazin-2-yl]amino]-1-hydroxy-3-sulfo-2-naphthalenyl]azo]phenyl]azo]-1',2'-dihydro-6'-hydroxy-4'-methyl-2'-oxo-, trichloride (9CI) (CA INDEX NAME)

PAGE 1-A

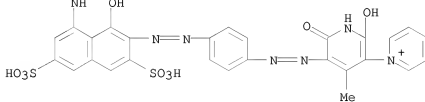
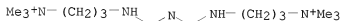
● 3 Cl⁻

PAGE 1-B



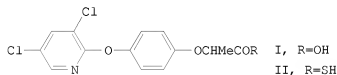
RN 88470-78-4 CAPLUS

CN 1,3'-Bipyridinium, 5'-[[4-[[8-[[4,6-bis[[3-(trimethylammonio)propyl]amino]-1,3,5-triazin-2-yl]amino]-1-hydroxy-3,6-disulfo-2-naphthalenyl]azo]phenyl]azo]-1',2'-dihydro-6'-hydroxy-4'-methyl-2'-oxo-, trichloride (9Cl) (CA INDEX NAME)

● 3 Cl⁻

L22 ANSWER 12 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
 AN 1983:156408 CAPLUS <<LOGINID::20080523>>
 DN 98:156408
 OREF 98:23669a,23672a
 TI Synergistic agent for the selective control of weeds, especially in crops
 IN Quadranti, Marco; Maag, Kurt
 PA Ciba-Geigy A.-G., Switz.
 SO Eur. Pat. Appl., 28 pp.
 CODEN: EPXXDW
 DT Patent
 LA German
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 69705	A1	19830112	EP 1982-810283	19820702
	EP 69705	B1	19850529		
	R: AT, BE, CH, DE, FR, GB, IT, LI, NL				
	AT 13478	T	19850615	AT 1982-810283	19820702
	ZA 8204820	A	19830427	ZA 1982-4820	19820707
	JP 58015903	A	19830129	JP 1982-119127	19820708
PRAI	CH 1981-4485	A	19810708		
	EP 1982-810283	A	19820702		
OS	MARPAT 98:156408				
GI					

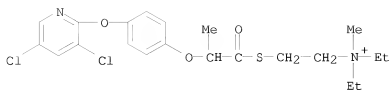


AB Synergistic herbicides for postemergence weed control in cereals were prepared by mixing 3-(4-isopropylphenyl)-1,1-dimethylurea [34123-59-6] or 3-(3-chloro-4-methylphenyl)-1,1-dimethylurea [15545-48-9] with 4-(3',5'-dichloropyridyl-2'-oxy)- α -phenoxypropionic acid (I) [60074-25-1] or its Me, Et, Pr, or Bu ester derivs. or with 4-(3',5'-dichloropyridyl-2'-oxy)- α -phenoxythiopropionic acid (II) [72132-05-9] or its ester derivs. at a 1:1-20:1, preferably 4:1-10:1, ratio and used preferably at 0.25-1.25 kg total active ingredient/ha. The herbicide formulations are described.

IT 72280-31-0
 RL: BIOL (Biological study)
 (synergist, for dimethylurea herbicides)

RN 72280-31-0 CAPLUS

CN Ethanaminium, 2-[[2-[4-[(3,5-dichloro-2-pyridinyl)oxy]phenoxy]-1-oxopropyl]thio]-N,N-diethyl-N-methyl-, iodide (9CI) (CA INDEX NAME)



● I⁻

L22 ANSWER 13 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1982:520110 CAPLUS <<LOGINID::20080523>>

DN 97:120110

OREF 97:19777a,19780a

TI QSAR in a series of muscarinic agents. Note IV. New pyridine and furan derivatives

AU Pratesi, P.; Villa, L.; Ferri, V.; De Micheli, C.; Grana, E.; Barbone, M. G. Santagostino; Silipo, C.; Vittoria, A.

CS Ist. Chim. Farm., Univ. Milano, Milan, Italy

SO Farmaco, Edizione Scientifica (1982), 37(6), 398-410

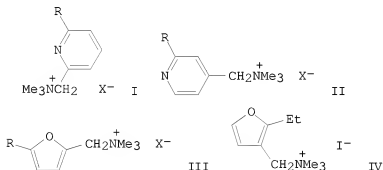
CODEN: FRPSAX; ISSN: 0430-0920

DT Journal

LA English

OS CASREACT 97:120110

GI



AB Five picolyltrimethylammonium salts I (R = Et, NO₂, or OMe) and II (R = Br or Cl), and 5 furfuryltrimethylammonium salts III (R = CH₂Cl, CH₂OH, NO₂, or CH:CH₂) and IV [83004-04-0] were prepared and their interaction with muscarinic receptors was studied in order to characterize the muscarinic receptor. Pharmacodynamic parameters (α , pD₂, pA₂) and the hydrophobic constant were used to clarify the ligand-receptor interactions and to elucidate structure-activity relations. The affinities of these compds. were expressed as pD₂ for mimetics and as pA₂ for partial agonists or competitive antagonists. The cumulative dose-response curve of all

agonists tested showed a slope similar to that of furmethide except for I iodide (R = Et) [83004-17-5]. Apparently, the biol. data for these new congeners was accurately predicted based on a previously published correlation equation.

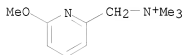
IT 83004-12-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of and muscarinic receptor binding by, QSAR in relation to)

RN 83004-12-0 CAPLUS

CN 2-Pyridinemethanaminium, 6-methoxy-N,N,N-trimethyl-, iodide (9CI) (CA INDEX NAME)



L22 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1981:191591 CAPLUS <<LOGINID::20080523>>

DN 94:191591

OREF 94:31333a,31336a

TI Convenient dealkylation of quaternary ammonium salts

AU Newkome, George R.; Majestic, Veronica K.; Sauer, Joe D.

CS Dep. Chem., Louisiana State Univ., Baton Rouge, LA, 70803, USA

SO Organic Preparations and Procedures International (1980), 12(6), 345-50

CODEN: OPPIAK; ISSN: 0030-4948

DT Journal

LA English

OS CASREACT 94:191591

AB Quaternary ammonium halides were dealkylated with Li(EtCHMe)3BH to give essentially quant. yields of the corresponding amines. Demethylation is favored over deethylation. Thus, dealkylation of PhN+Et2Me I- at 25° gave 82% PhNEt2 and 7% PhNMeEt.

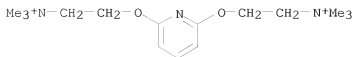
IT 29449-87-4 29460-15-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(demethylation of, reagent for)

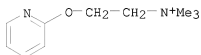
RN 29449-87-4 CAPLUS

CN Ethanaminium, 2,2'-(2,6-pyridinediylbis(oxy))bis[N,N,N-trimethyl-, diiodide (9CI) (CA INDEX NAME)



● 2 I⁻

RN 29460-15-9 CAPLUS
 CN Ethanaminium, N,N,N-trimethyl-2-(2-pyridinyloxy)-, iodide (9CI) (CA INDEX NAME)



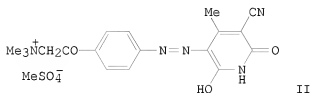
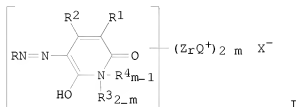
● I⁻

L22 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
 AN 1980:587740 CAPLUS <<LOGINID::20080523>>
 DN 93:187740
 OREF 93:29943a,29946a
 TI Cationic 5-arylazo-6-hydroxypyridone-2 dyes
 IN Entschel, Roland; Mueller, Curt; Steinemann, Willy
 PA Sandoz A.-G., Switz.
 SO U.S., 34 pp. Cont.-in-part of U.S. Ser. No. 824,298, abandoned.
 CODEN: USXXAM
 DT Patent
 LA English
 FAN.CNT 16

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4213898	A	19800722	US 1973-400527	19730925
	CH 503781	A	19710228	CH 1968-503781	19680515
	CH 506592	A	19710430	CH 1968-506592	19680813
	BR 6908780	D0	19730109	BR 1969-208780	19690514
	FR 2008615	A5	19700123	FR 1969-15876	19690516
	FR 2008615	B1	19731130		
	ES 377393	A2	19720916	ES 1970-377393	19700311
	US 4032532	A	19770628	US 1973-337167	19730301
	PRAI CH 1968-7218	A	19680515		
	CH 1968-11581	A	19680802		
PRAI	CH 1968-12136	A	19680813		
	US 1969-824298	A2	19690513		

US 1969-810014 A 19690324
US 1969-824297 A2 19690513

GI



AB Water-soluble dyes (I) giving fast shades on acrylic fibers are prepared, where R = aromatic carbocyclic or heterocyclic group, R¹ = H or CN, R² = optionally substituted alkyl, aryl, or heterocyclyl, R³ = H or optionally substituted hydrocarbaryl, heterocyclyl, or amino, R⁴ = quaternized N-containing heterocyclyl, m = 1 or 2, Z = divalent bridging group, r = 0 or 1, Q⁺ = optionally substituted ammonium, hydrazinium or quaternized N-containing heterocyclyl, and X⁻ = anion. Thus, 4-amino-*o*-(dimethylamino)acetophenone [28799-80-6] was diazotized and coupled with 5-cyano-2,6-dihydroxy-4-methylpyridine [5444-02-0], and the resulting azo compound [37710-82-0] was treated with Me₂SO₄ to give II [30506-77-5], a greenish yellow dye for acrylic fibers. Numerous other I were similarly prepared

IT 30506-77-5P

RL: PREP (Preparation)

(manufacture of, as dye for acrylic fibers)

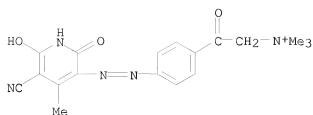
RN 30506-77-5 CAPLUS

CN Benzeneethanaminium, 4-[(5-cyano-1,2-dihydro-6-hydroxy-4-methyl-2-oxo-3-pyridinyl)azo]-N,N,N-trimethyl-β-oxo-, methyl sulfate (salt) (9CI)
(CA INDEX NAME)

CM 1

CRN 47488-32-4

CMF C18 H20 N5 O3



CM 2

CRN 21228-90-0

CMF C H3 O4 S

Me-O-SO₃⁻

L22 ANSWER 16 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1980:41772 CAPLUS <<LOGINID::20080523>>

DN 92:41772

OREF 92:6969a,6972a

TI Herbicidal pyridyloxyphenoxy- α -propionic acid aminoalkyl esters

IN Schurter, Rolf; Rempfler, Hermann; Boehner, Beat

PA Ciba-Geigy A.-G., Switz.

SO Eur. Pat. Appl., 35 pp.

CODEN: EPXXDW

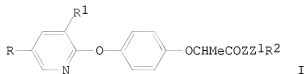
DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 3313	A1	19790808	EP 1979-100127	19790117
	EP 3313	B1	19810107		
	R: BE, CH, DE, FR, GB, IT, NL				
	US 4213774	A	19800722	US 1979-5538	19790122
	CS 203942	B2	19810331	CS 1979-507	19790123
	RO 76447	A1	19810330	RO 1979-96388	19790125
	CA 1100965	A1	19810512	CA 1979-320291	19790125
	IL 56498	A	19820730	IL 1979-56498	19790125
	AU 7943698	A	19790802	AU 1979-43698	19790126
	AU 527702	B2	19830317		
	BR 7900495	A	19790828	BR 1979-495	19790126
	JP 54109982	A	19790829	JP 1979-8653	19790126
	JP 02017545	B	19900420		
	ZA 7900336	A	19800227	ZA 1979-336	19790126
	DD 141775	A5	19800521	DD 1979-210662	19790126
	AT 7900601	A	19820915	AT 1979-601	19790126
	AT 370587	B	19830411		
	HU 24367	A2	19830228	HU 1979-CI1900	19790126
	HU 181862	B	19831128		

	AT 8200208	A	19850715	AT 1982-208	19820121
	AT 379802	B	19860310		
PRAI	CH 1978-928		19780127		
GI	AT 1979-601	A	19790126		

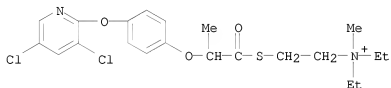


AB The title compds. I [R = halogen, CF₃; R₁ = H, halogen, CF₃; R₂ = (substituted) NH₂, NH₃⁺, or pyridinium; Z = O, S; Z₁ = alkylene, oxaalkylene] were prepared for use as herbicides (test data tabulated). Thus, II reacted with HOCH₂CH₂NMe₂ in CH₂Cl₂-Et₃N to give I (R = R₁ = Cl, Z = O, Z₁ = CH₂CH₂, R₂ = Me₂N).

IT 72280-31-0P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation and herbicidal activity of)

RN 72280-31-0 CAPLUS

CN Ethanaminium, 2-[[2-[4-[(3,5-dichloro-2-pyridinyl)oxy]phenoxy]-1-oxopropyl]thio]-N,N-diethyl-N-methyl-, iodide (9CI) (CA INDEX NAME)

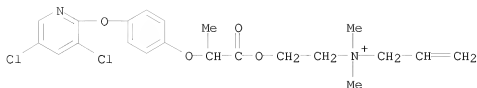


● I⁻

IT 72280-37-6P 72280-38-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

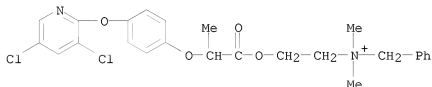
RN 72280-37-6 CAPLUS

CN 2-Propen-1-aminium, N-[2-[2-[4-[(3,5-dichloro-2-pyridinyl)oxy]phenoxy]-1-oxopropoxy]ethyl]-N,N-dimethyl-, chloride (9CI) (CA INDEX NAME)



RN 72280-38-7 CAPLUS

CN Benzenemethanaminium, N-[2-[2-[4-[(3,5-dichloro-2-pyridinyl)oxy]phenoxy]-1-oxopropoxy]ethyl]-N,N-dimethyl-, chloride (9CI) (CA INDEX NAME)



L22 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1979:551075 CAPLUS <<LOGINID::20080523>>

DN 91:151075

OREF 91:24225a,24228a

TI A quantitative aspect of charge-transfer phenomenon in the biological activity of hallucinogens, local anesthetics and nicotinic agents

AU Gupta, S. P.; Singh, P.

CS Dep. Chem., Birla Inst. Technol. Sci., Pilani, 333 031, India

SO Proceedings - Indian Academy of Sciences, Section A (1979), 88A(Pt. 1, No. 3), 171-7

CODEN: PISAA7; ISSN: 0370-0089

DT Journal

LA English

AB The qual. electronic structure-activity relations suggesting that hallucinogens, local anesthetics, and nicotinic agents exert their biol. effects through the formation of charge-transfer complexes with the receptors were tested statistically. The statistical test supported the suggestion and further suggested that along with the charge-transfer mechanism a secondary binding is also involved in the activity of nicotinic agents.

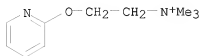
IT 71601-72-4

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); BIOL (Biological study)
(nicotinic activity of, structure in relation to)

RN 71601-72-4 CAPLUS

CN Ethanaminium, N,N,N-trimethyl-2-(2-pyridinyloxy)- (CA INDEX NAME)



L22 ANSWER 18 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1977:469735 CAPLUS <<LOGINID::20080523>>

DN 87:69735

OREF 87:11117a,11120a

TI 2,6-Dihydroxy-3-cyano-4-methylpyridine-containing azo dyes which contain a functional amino group

IN Ramanathan, Visvanathan

PA Ciba-Geigy A.-G., Switz.

SO U.S., 16 pp.

CODEN: USXXAM

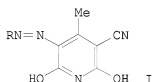
DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
PI	US 3966706	A	19760629	US 1973-395304	19730907
PRAI	US 1969-827960	A1	19690526		
	US 1971-110240	A1	19710127		

GI

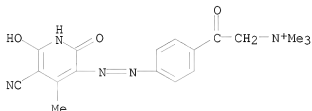


AB Title dyes of general structure I, where R is an aromatic or heterocyclic residue containing an amino group that may be quaternized, give fast yellow or orange dyeings on acrylic fibers. Typical dyes, all prepared by conventional diazo coupling reactions, include I (R = Cl- p-Me3N+CH2COC6H4) [25826-12-4], I [R = 6-[(dimethylamino)methyl]-2-benzothiazolyl] [25737-76-2], and I [R = 3-[(1-methylpyridinium-3-ylcarbonyl)amino]phenyl] [30205-18-6].

IT 25826-12-4
RL: USES (Uses)

(dye, for acrylic fibers, preparation of)

RN 25826-12-4 CAPLUS
 CN Benzeneethanaminium, 4-[(5-cyano-1,2-dihydro-6-hydroxy-4-methyl-2-oxo-3-pyridinyl)azo]-N,N,N-trimethyl-β-oxo-, chloride (9CI) (CA INDEX NAME)

● Cl⁻

L22 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1975:74435 CAPLUS <<LOGINID::20080523>>

DN 82:74435

OREF 82:11911a,11914a

TI Basic azo dyes

IN Entschel, Roland; Mueller, Curt; Steinemann, Willy

PA Sandoz Ltd.

SO Patentschrift (Switz.), 6 pp.

CODEN: SWXXAS

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CH 553241	A	19740830	CH 1971-13987	19691017
PRAI	CH 1971-13987	A	19691017		

GI For diagram(s), see printed CA Issue.

AB Cationic azo dyes (I, R, R1 = H, Me; Z = COCH2, CONHCH2CH2CH2; X = Cl, MeSO4) and unquaternized derivs. were prepared and dyed acrylic and poly(vinylidene cyanide) fibers fast greenish yellow shades. Thus, 4-H2NC6H4COCH2NMe2 [28799-80-6] was diazotized and coupled with 2,6-dihydroxy-4-methylpyridine [4664-16-8], the azo compound isolated, and methylated with Me2SO4 to give cationic azo dye I(R =R1 = H, Z = p-COCH2, X = MeSO4) [53461-12-4]. The other I was similarly prepared

IT 53461-12-4P

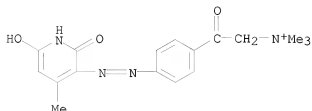
RL: IMF (Industrial manufacture); PREP (Preparation)
 (preparation of)

RN 53461-12-4 CAPLUS

CN Benzeneethanaminium, 4-[(1,2-dihydro-6-hydroxy-4-methyl-2-oxo-3-pyridinyl)azo]-N,N,N-trimethyl-β-oxo-, methyl sulfate (salt) (9CI)
 (CA INDEX NAME)

CM 1

CRN 53461-11-3
CMF C17 H21 N4 O3



CM 2

CRN 21228-90-0
CMF C H3 O4 S

Me-O-SO₃⁻

L22 ANSWER 20 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1970:530899 CAPLUS <<LOGINID::20080523>>

DN 73:130899

OREF 73:21329a,21332a

TI Pesticidal substituted aminothioethoxy pyridines

IN Zielinski, James

PA Esso Research and Engineering Co.

SO U.S., 18 pp.

CODEN: USXXAM

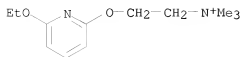
DT Patent

LA English

FAN.CNT 1

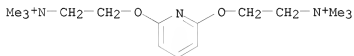
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3535328	A	19701020	US 1967-664944	19670901
PRAI	US 1967-664944	A	19670901		
AB	Mono- and polysubstituted pyridine derivs., useful as pesticides were prepared by 9 different methods. Thus, 2-chloro-6-benzylthiopyridine was prepared by adding NaOEt to PhCH ₂ SH and refluxing the product with 2,6-dichloropyridine. More than 150 derivs. of substituted pyridine derivs. were prepared				
IT	29449-83-0P	29449-87-4P	29450-03-1P		
	29450-20-2P	29460-15-9P	29460-43-3P		
	29476-03-7P				
	RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)				
RN	29449-83-0	CAPLUS			
CN	Ammonium, [2-[(6-ethoxy-2-pyridyl)oxy]ethyl]trimethyl-, iodide (8CI) (CA				

INDEX NAME)



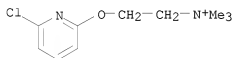
RN 29449-87-4 CAPLUS

CN Ethanaminium, 2,2'-[2,6-pyridinediylbis(oxy)]bis[N,N,N-trimethyl-, diiodide (9CI) (CA INDEX NAME)



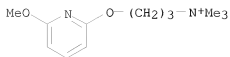
RN 29450-03-1 CAPLUS

CN Ammonium, [2-[(6-chloro-2-pyridyl)oxy]ethyl]trimethyl-, iodide (8CI) (CA INDEX NAME)



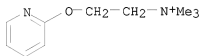
RN 29450-20-2 CAPLUS

CN Ammonium, [3-[(6-methoxy-2-pyridyl)oxy]propyl]trimethyl-, iodide (8CI) (CA INDEX NAME)



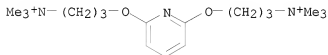
RN 29460-15-9 CAPLUS

CN Ethanaminium, N,N,N-trimethyl-2-(2-pyridinyloxy)-, iodide (9CI) (CA INDEX NAME)



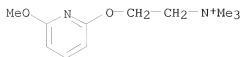
RN 29460-43-3 CAPLUS

CN Ammonium, [2,6-pyridinediylbis(oxytrimethylene)]bis[trimethyl-, diiodide (8CI) (CA INDEX NAME)



RN 29476-03-7 CAPLUS

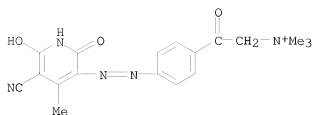
CN Ammonium, [2-[(6-methoxy-2-pyridyl)oxy]ethyl]trimethyl-, iodide (8CI) (CA INDEX NAME)



● I⁻

L22 ANSWER 21 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
 AN 1970:510871 CAPLUS <<LOGINID::20080523>>
 DN 73:110871
 OREF 73:18055a,18058a
 TI Azo dyes
 IN Ramanathan, Visvanathan
 PA CIBA Ltd.
 SO Ger. Offen., 55 pp.
 CODEN: GWXXBX
 DT Patent
 LA German
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 1927213	A	19691204	DE 1969-1927213	19690529
	CH 557857	A	19750115	CH 1968-8113	19680531
	FR 2014146	A5	19700417	FR 1969-16780	19690522
	SU 433691	A3	19740625	SU 1969-1334340	19690528
	BE 733834	A	19691201	BE 1969-733834	19690530
	NL 6908284	A	19691202	NL 1969-8284	19690530
	ES 367877	A1	19710416	ES 1969-367877	19690530
	GB 1277090	A	19720607	GB 1969-1277090	19690530
PRAI	CH 1968-8113	A	19680531		
	CH 1969-4967	A	19690401		
GI	For diagram(s), see printed CA Issue.				
AB	The title compds., I and II, yellow to orange dyes for polyacrylonitrile fibers, are prepared by coupling 2,6-dihydroxy-3-cyano-4-methylpyridine (III) with diazotized amines. Thus, III was coupled with diazotized 4-H2NC6H4COCH2NMe3+Cl- to give a yellow dye, also prepared from I (R = p-COCH2C1) and Me3N. Similarly were prepared II and 2 other I.				
IT	25826-12-4P				
	RL: IMF (Industrial manufacture); PREP (Preparation) (preparation of)				
RN	25826-12-4 CAPLUS				
CN	Benzeneethanaminium, 4-[(5-cyano-1,2-dihydro-6-hydroxy-4-methyl-2-oxo-3-pyridinyl)azo]-N,N,N-trimethyl-β-oxo-, chloride (9CI) (CA INDEX NAME)				



● Cl⁻

L22 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN

AN 1969:484689 CAPLUS <<LOGINID::20080523>>

DN 71:84689

OREF 71:15775a,15778a

TI Molecular orbital calculations on a new series of substituted-phenyl choline ethers

AU Crow, James; Wassermann, Otmar; Holland, William C.

CS Sch. of Med., Univ. of Mississippi, Jackson, MS, USA

SO Journal of Medicinal Chemistry (1969), 12(5), 764-6

CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

AB In addition to the onium head, it has been suggested that the electron d. at some other points in the mol. of phenyl and substituted-phenyl choline ethers contribute to the intensity of nicotine-like activity. Simple Hueckel M.O. calcs. revealed that charge ds. in the remainder of the mol. could not be correlated with pharmacologic activity. However, superdelocalizability at ring positions 2 and 6 and the energy of the highest occupied M.O. showed good parallelism with biologic activity. It was suggested that the aromatic ring may interact with the receptor by forming a charge-transfer complex.

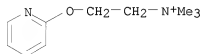
IT 25077-27-4

RL: PRP (Properties)

(mol. orbitals of)

RN 25077-27-4 CAPLUS

CN Ammonium, trimethyl[2-(2-pyridyloxy)ethyl]-, bromide (8CI) (CA INDEX NAME)



● Br⁻

